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Bulk photovoltaic effect in $\text{CH}_3\text{NH}_3\text{PbI}_3$ and $\text{CH}_3\text{NH}_3\text{PbI}_{3-x}\text{Cl}_x$
NATHAN Z. KOOSHER, FAN ZHENG, HIROYUKI TAKENAKA, FENGGONG WANG, ANDREW M. RAPPE, Univ of Pennsylvania — The power conversion efficiency of methylammonium lead iodide (MAPbI_3)-based organometal halide perovskites has increased to nearly 20%, fueling interest in understanding the mechanism of its photovoltaic effect. High open-circuit photovoltages and I/V hysteresis curves have been experimentally measured for these materials, which suggest that the bulk photovoltaic effect (BPVE) could be in operation. Shift current is a main mechanism of the BPVE in ferroelectric perovskite oxides, and thus in our work, we calculate the shift current response of MAPbI_3 and $\text{MAPbI}_{3-x}\text{Cl}_x$. We find that MAPbI_3 and $\text{MAPbI}_{3-x}\text{Cl}_x$ have shift current responses about three times larger than that of BiFeO_3 . Specifically, the shift current response is enhanced when the molecular dipoles from the methylammonium molecules are aligned in the same direction and when Cl is substituted into the lattice. Because of the large shift current response, the BPVE may play a role in enhancing the performance of the solar cells.

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